Process Modeling of Composites by Resin Transfer Molding: Sensitivity Analysis for Non-Isothermal Considerations

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Abstract

The resin transfer molding (RTM) manufacturing process consists of either of two considerations. The first is the fluid flow analysis where tracking of the flow fronts are of primary importance, and the second is the combined multi-disciplinary flow/thermal analysis, where kinetics and cure need to be accounted for in the process modeling stages. In the combined multi-disciplinary flow/thermal analysis, viscosity is a function of temperature. The so-called continuous sensitivity formulations are developed for the latter case of non-isothermal process modeling of composites manufactured by RTM to predict, analyze, and optimize the manufacturing process. Attention is focused on developments for non-isothermal process modeling simulations, and numerical illustrative examples are presented for the sensitivity analysis of structural composites manufactured by RTM.

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1. Introduction

Process modeling employing resin transfer molding (RTM) to manufacture complex structural geometries involves the injection of a polymer resin into a porous fibrous preform conforming to the geometry of the manufactured part. The mold is normally at a higher temperature than the resin; therefore, the analysis of this process requires accounting for both the flow and thermal-kinetic equations. The solutions of these equations provide the flow front position, temperature, and cure information to the analyst. After the results from the numerical analysis are obtained, a systematic process of optimization is performed with the assistance of the continuous sensitivity equation, thereby avoiding heuristic trial-and-error methods.

The thermal processes involved in the resin transfer molding (RTM) model are investigated in this report. The non-isothermal RTM analyses have been previously investigated in references [1–4]. Modeling of both temperature and cure are important because the viscosity of the resin is sensitive to both of these factors. Before reaction of the polymer resin occurs, the resin is temperature sensitive; but after polymerization begins, the resin is cure sensitive [1]. Although the continuous sensitivity equation (CSE) has been previously applied under isothermal conditions [5,6], the aim of this report is to extend this to non-isothermal situations for the first time. Besides the development of the CSE for non-isothermal RTM, the fill time sensitivity with respect to the inlet temperature is also described.

The CSE for mold filling is formulated for process modeling of composites that take into account non-isothermal considerations. The thermal model is first presented and solved numerically by coupling with the flow model. This thermal model includes solutions for temperature and cure. The CSE for non-isothermal RTM filling is presented next, followed by the CSE for the temperature and cure sensitivity considerations. Finally, illustrative numerical results are presented for two sample axi-symmetric geometries, which includes

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verification of the fill time sensitivity for a sensitivity parameter of inlet temperature.

2. Non-Isothermal Resin Transfer Molding

In this section, the temperature and cure model equations are described for non-isothermal RTM filling. Non-isothermal effects are an important consideration in many manufacturing process modeling applications employing RTM. Heat is transferred via various mechanisms of transport during a mold filling process. These include convection from the mold walls, advection from the fluid, radiation to and from the mold, and heat generated by the exothermic curing process of the resin. For non-isothermal considerations, the independent parameters include conductivity, permeability, viscosity, and inlet pressure or flow rate. The dependent variables are the temperature and amount of resin cure.

The first step to developing the so-called continuous sensitivity equations for the non-isothermal filling process is to begin from the governing model differential equations. By assuming that the fiber and resin temperatures are at the same equilibrium temperature inside a small control volume [1], the energy balance can be written as

$$\rho c_p \frac{\partial T}{\partial t} + \rho_r c_{pr}(\mathbf{u} \cdot \nabla T) = \nabla \cdot k\nabla T + \Phi \dot{G} \tag{1}$$

where $\dot{G}$ is the heat generated from the curing of the resin and Φ is the volume of fiber fraction. The average material properties are computed by

$$\rho c_p = \Phi \rho_r c_{pr} + (1 - \Phi)\rho_f c_{pf}$$

$$k = k_s + k_D \tag{2}$$

$$k_s = \Phi k_r + (1 - \Phi)k_f$$

where the subscripts f and r denote fiber and resin properties, respectively. k_D is the thermal dispersion conductivity due to mechanical dissipation. The computation for the

effective conductivity is given as

$$k_{eff} = \frac{k_f k_r}{k_f w_r + k_r w_f} \tag{3}$$

where

$$w_f = 1 - w_r$$
$$w_r = \frac{\frac{\Phi}{\rho_f}}{\frac{\Phi}{\rho_f} + \frac{(1-\Phi)}{\rho_r}} \tag{4}$$

Equation (1) represents the equilibrium temperature model used for developing the finite element equations that can then be readily implemented and solved numerically. The boundary conditions for the non-isothermal mold-filling process are given as

$$T = T_w \text{ at mold wall}$$
$$T = T_{r0} \text{ during filling, at inlet}$$
$$k\frac{\partial T}{\partial n} = (1 - \Phi)\rho_r c_{pr} \mathbf{u} \cdot \mathbf{n}(T_{f0} - T) \text{ at resin front} \tag{5}$$
$$T(t = 0) = T_w$$

where T_r is the temperature of the resin, T_w is the wall temperature, and $\mathbf{n}$ is the direction normal to the resin flow front. The initial conditions·for solving the temperature problem are given as

$$T_r(t = 0) = T_{r0} \text{ and } T_f(t = 0) = T_w \tag{6}$$

where T_f is the temperature of the fibrous preform. Another thermal computation involved in non-isothermal RTM filling is cure. The curing analysis begins with the species mass balance and is given as

$$\Phi\frac{\partial \alpha}{\partial t} + \mathbf{u} \cdot \nabla\alpha = \Phi R_\alpha \tag{7}$$

Here, α is the degree of cure, $\mathbf{u}$ is the velocity field, and R_α is the rate of chemical reaction. The boundary conditions for the cure problem are given by

$$\alpha = 0 \text{ during filling, at the model inlet(s)} \tag{8}$$

The initial conditions are given by

$$\alpha(t = 0) = 0 \tag{9}$$

Since curing is an exothermic process, the heat generated is calculated with the following equation [2-4]

$$\dot{G} = H_R R_\alpha \tag{10}$$

where the term R_α is defined as

$$R_\alpha = (K_1 + K_2 \alpha^{n1})(1 - \alpha)^{n2} \tag{11}$$

and H_R is the heat of reaction per unit volume for the pure resin. The constants K_1 and K_2 are assumed as

$$
\begin{aligned}
K_1 &= A_1 exp\left(-\frac{E_1}{RT}\right) \\
K_2 &= A_2 exp\left(-\frac{E_2}{RT}\right)
\end{aligned}
\tag{12}
$$

where A_1, A_2, E_1, E_2, n_1, and n_2 are the kinetic constants determined experimentally for each resin used. The resin viscosity is a function of the degree of cure and temperature. The model used for the viscosity is given as [7]

$$\mu = A_\mu exp\left(\frac{E_\mu}{RT}\right)\left(\frac{\alpha_g}{\alpha_g - \alpha}\right)^{A+B\alpha} \tag{13}$$

which is used in conjunction with the implicit filling technique due to Mohan et al. [8]. This method has proven to be an effective approach for solving this class of problems.

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Continuing with the development of the heat transfer finite element equations, begin with the thermal equilibrium model in equation (1) and employ the method of weighted residuals. Thus,

$$\int_\Omega \mathbf{W}^T \left[\rho c_p \frac{\partial T}{\partial t} + \rho_r c_{pr}(\mathbf{u} \cdot T) - \nabla \cdot k\nabla T - \Phi \dot{G} \right] d\Omega = 0 \qquad (14)$$

Separating the terms and integrating by parts yields

$$\int_\Omega \mathbf{W}^T \rho c_p \frac{\partial T}{\partial t} \, d\Omega + \int_\Omega \mathbf{W}^T \rho_r c_{pr}(\mathbf{u} \cdot \nabla T) \, d\Omega - \int_\Gamma \mathbf{W}^T (k\nabla T \cdot \mathbf{n}) \, d\Gamma +$$
$$\int_\Omega \nabla \mathbf{W}^T k\nabla T \, d\Omega - \int_\Omega \mathbf{W}^T \Phi \dot{G} \, d\Omega = 0 \qquad (15)$$

Defining the weighting functions $\mathbf{W}$ to be the Streamline Upwind Petrov-Galerkin (SUPG) weighting functions $\mathbf{N} + \lambda(\mathbf{u} \cdot \nabla \mathbf{N})$ and interpolating for T yields

$$\mathbf{W} = \mathbf{N} + \lambda(\mathbf{u} \cdot \nabla \mathbf{N})$$
$$\mathbf{T} = \sum_{i=1}^{\text{num. nodes}} W_i T_i \qquad (16)$$

where i represents the associated node numbers. The heat flux, $\mathbf{q}$, is defined as

$$k\nabla T \cdot \mathbf{n} = -\mathbf{q} \cdot \mathbf{n} \qquad (17)$$

Substituting equation (16) and equation (17) into equation (15) yields

$$\left[\int_\Omega W_i \rho c_p N_i \, d\Omega \right] \frac{\partial T_i}{\partial t} + \left[\int_\Omega W_i \rho_r c_{pr}(\mathbf{u} \cdot \nabla N_i) \, d\Omega \right] T_i + \left[\int_\Omega \nabla W_i k\nabla N_i \, d\Omega \right] T_i$$
$$= \int_\Gamma W_i(k\nabla T \cdot \mathbf{n}) \, d\Gamma + \int_\Omega W_i \Phi \dot{G} \, d\Omega \qquad (18)$$

For the temperature analysis, the resulting semi-discretized equation is thus obtained as

$$\mathbf{C}\dot{\mathbf{T}} + (\mathbf{K}_{\text{ad}} + \mathbf{K}_{\text{cond}})\mathbf{T} = \mathbf{Q}_{\mathbf{q}} + \mathbf{Q}_{\dot{\mathbf{G}}} \qquad (19)$$

where the terms in equation (19) are defined as

$$\mathbf{C} = \int_\Omega \mathbf{W}^T \rho c_p \mathbf{N}\, d\Omega$$

$$\mathbf{K_{ad}} = \int_\Omega \mathbf{W}^T \rho c_{pr} (\mathbf{u} \cdot \mathbf{B}_N)\, d\Omega$$

$$\mathbf{K_{cond}} = \int_\Omega \mathbf{B}_W^T k \mathbf{B}_N\, d\Omega \tag{20}$$

$$\mathbf{Q_q} = \int_\Gamma \mathbf{W}^T (-\mathbf{q} \cdot \mathbf{n})\, d\Gamma$$

$$\mathbf{Q_{\dot{G}}} = \int_\Omega \mathbf{W}^T \Phi \dot{G}\, d\Omega$$

The time discretization for the temperature analysis is employed, for an arbitrary θ, as

$$\dot{\mathbf{T}}_\theta = \frac{\mathbf{T}_{n+1} - \mathbf{T}_n}{\Delta t} \tag{21}$$

The cure model equation is also solved using the finite element method. Applying the method of weighted residuals on the species mass balance in equation (7) yields

$$\int_\Omega \mathbf{W}^T \left(\Phi \frac{\partial \alpha}{\partial t} + \mathbf{u} \cdot \nabla \alpha - \Phi R_\alpha \right) d\Omega = 0 \tag{22}$$

Subsequently, separating terms and integrating by parts yields

$$\int_\Omega \mathbf{W}^T \Phi \frac{\partial \alpha}{\partial t}\, d\Omega + \int_\Omega \mathbf{W}^T \mathbf{u} \cdot \nabla \alpha\, d\Omega - \int_\Omega \Phi R_\alpha\, d\Omega = 0 \tag{23}$$

As in the temperature problem, the weighting functions $\mathbf{W}$ are defined as the SUPG weighting functions $\mathbf{N} + \lambda(\mathbf{u} \cdot \nabla \mathbf{N})$ and interpolating for α yields

$$\mathbf{W} = \mathbf{N} + \lambda(\mathbf{u} \cdot \nabla \mathbf{N})$$

$$\alpha = \sum_{i=1}^{\text{num. nodes}} W_i \alpha_i \tag{24}$$

Rewriting equation (23) in the semi-discretized form results in

$$\mathbf{C}\dot{\alpha} + \mathbf{K}\alpha = \mathbf{Q_{R_\alpha}} \tag{25}$$

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where the terms in equation (25) are defined as

$$C = \int_\Omega \Phi W^T N \, d\Omega$$

$$K = \int_\Omega W^T (u \cdot B_N) \, d\Omega \tag{26}$$

$$Q_{R_\alpha} = \int_\Omega \Phi W^T R_\alpha \, d\Omega$$

The time discretization for the cure analysis is employed, for an arbitrary θ, as

$$\dot{\alpha}_\theta = \frac{\alpha_{n+1} - \alpha_n}{\Delta t} \tag{27}$$

A more detailed discussion of the non-isothermal RTM computational analysis can be found in Ngo et al. [9].

3. Sensitivity Analysis of Non-Isothermal Resin Transfer Molding

In this section, the continuous sensitivity equation for non-isothermal RTM filling, temperature, and cure are defined. The computational procedure for the non-isothermal RTM filling problem is described, along with some illustrative results from an example axi-symmetric model. Finally, the fill time sensitivity with respect to the inlet temperature is discussed and verified with the use of an additional axi-symmetric example.

3.1 RTM Filling Sensitivity

For the non-isothermal pressure sensitivity calculation, viscosity is a function of temperature and cure (i.e., $\mu(T, \alpha)$). The sensitivity equation for RTM filling is given by the following

semi-discretized equation as

$$\frac{\partial \mathbf{K}}{\partial p}\mathbf{P} + \mathbf{K}\mathbf{S_P} = \mathbf{S_q} \tag{28}$$

where p is the specified sensitivity parameter. Equation (28) is the same CSE used in isothermal filling simulations and the derivation thereof is given in the aforementioned isothermal references [5,6]. The terms $\frac{\partial \mathbf{K}}{\partial p}$, $\mathbf{K}$, and $\mathbf{S_q}$ from equation (28) are defined as

$$\frac{\partial \mathbf{K}}{\partial p} = \int_\Omega \mathbf{B^T}\frac{\partial \bar{K}}{\partial p}\frac{1}{\mu}\mathbf{B}\,d\Omega + \int_\Omega \mathbf{B^T}\bar{K}\left(-\frac{1}{\mu^2}\right)\frac{\partial \mu}{\partial p}\mathbf{B}\,d\Omega$$

$$\mathbf{K} = \int_\Omega \mathbf{B^T}\frac{\bar{K}}{\mu}\mathbf{B}\,d\Omega$$

$$\mathbf{S_q} = \int_\Gamma \mathbf{N^T}\frac{\partial \bar{K}}{\partial p}\frac{1}{\mu}\cdot \nabla P \cdot \mathbf{n}\,d\Gamma + \int_\Gamma \mathbf{N^T}\bar{K}\frac{\partial}{\partial p}\left(\frac{1}{\mu}\right)\cdot \nabla P \cdot \mathbf{n}\,d\Gamma + \int_\Gamma \mathbf{N^T}\frac{\bar{K}}{\mu}\cdot \nabla S_P \cdot \mathbf{n}\,d\Gamma$$

$$\tag{29}$$

In equation (29), $\bar{K}$ is the permeability tensor of the fiber preform. With the viscosity defined as a function of temperature and cure, this leads to an additional term in the non-isothermal RTM filling continuous sensitivity equation, namely $\frac{\partial}{\partial p}\left(\frac{1}{\mu(T,\alpha)}\right)$

$$\frac{\partial \mathbf{K}}{\partial p} = \int_\Omega \mathbf{B^T}\frac{\partial \bar{K}}{\partial p}\frac{1}{\mu}\mathbf{B}\,d\Omega + \int_\Omega \mathbf{B^T}\bar{K}\left(-\frac{1}{\mu^2}\right)\frac{\partial \mu(T,\alpha)}{\partial p}\mathbf{B}\,d\Omega \tag{30}$$

where $\frac{\partial \mu(T,\alpha)}{\partial p}$ is defined as

$$\frac{\partial \mu(T(p),\alpha(p);p)}{\partial p} = \frac{\partial \mu}{\partial p} + A_\mu\left(\frac{\alpha_g}{\alpha_g - \alpha}\right)^{A+B\alpha}\left[-\frac{E_\mu}{RT^2}e^{\left(\frac{E_\mu}{RT}\right)}\right]\frac{\partial T}{\partial p}$$

$$+ A_\mu e^{\left(\frac{E_\mu}{RT}\right)}\left[\left(\frac{\alpha_g}{\alpha_g - \alpha}\right)^{A+B\alpha}\left[-\frac{A+B\alpha}{\alpha_g - \alpha} + B\ln\left(\frac{\alpha_g}{\alpha_g - \alpha}\right)\right]\right]\frac{\partial \alpha}{\partial p} \tag{31}$$

Note, that for $\mu = $ constant and $\frac{\partial \mu}{\partial p} = 0$ where $\mu \neq p$, it will yield the same results as the isothermal model equation. In the non-isothermal filling simulations the temperatures are also computed, which allows for the solution of the temperature sensitivity equations.

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3.2 RTM Temperature Sensitivity

The temperature sensitivity is evaluated by taking the partial derivative of equation (1) with respect to the sensitivity parameter p.

$$\frac{\partial}{\partial p}\left[\rho c_p \frac{\partial T}{\partial t} + \rho_r c_{pr}(\mathbf{u}\cdot\nabla T)\right] = \frac{\partial}{\partial p}\left[\nabla\cdot k\nabla T + \Phi\dot{G}\right] \tag{32}$$

This results in

$$\frac{\partial}{\partial p}(\rho c_p)\frac{\partial T}{\partial t} + \rho c_p\frac{\partial S_T}{\partial t} + \frac{\partial}{\partial p}(\rho c_p)(\mathbf{u}\cdot\nabla T) + \rho_r c_{pr}\frac{\partial}{\partial p}(\mathbf{u}\cdot\nabla T)$$
$$= \nabla\cdot\frac{\partial k}{\partial p}\nabla T + \nabla\cdot k\nabla S_T + \frac{\partial\Phi}{\partial p}\dot{G} + \Phi\frac{\partial\dot{G}}{\partial p} \tag{33}$$

where the temperature sensitivity is defined as $S_T \equiv \frac{\partial T}{\partial p}$. Moving all the terms in equation (33) to the left hand side and applying the method of weighted residuals yields

$$\int_\Omega \mathbf{W}^T\left[\frac{\partial}{\partial p}(\rho c_p)\frac{\partial T}{\partial t} + \rho c_p\frac{\partial S_T}{\partial t} + \frac{\partial}{\partial p}(\rho c_p)(\mathbf{u}\cdot\nabla T) + \rho_r c_{pr}\frac{\partial}{\partial p}(\mathbf{u}\cdot\nabla T)\right]d\Omega-$$
$$\int_\Omega \mathbf{W}^T\left[\nabla\cdot\frac{\partial k}{\partial p}\nabla T + \nabla\cdot k\nabla S_T + \frac{\partial\Phi}{\partial p}\dot{G} + \Phi\frac{\partial\dot{G}}{\partial p}\right]d\Omega = 0 \tag{34}$$

Before deriving the finite element equations, the partial derivative of the boundary conditions for the temperature analysis need to be computed. For the temperature analysis, equation (33), the boundary conditions are as follows:

$$S_T = \frac{\partial T_w}{\partial p} \text{ at the mold wall}$$

$$S_T = \frac{\partial T_{r0}}{\partial p} \text{ during filling, at mold inlet} \tag{35}$$

$$k\frac{\partial S_T}{\partial n} = \frac{\partial}{\partial p}\left((1-\Phi)\rho_r c_{pr}(\mathbf{u}\cdot\mathbf{n})(T_{f0}-T)\right) \text{ at resin flow front}$$

After applying the Green-Gauss theorem to convert the volume integral to a surface integral,

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the temperature sensitivity equation is given as

$$\int_{\Omega} \mathbf{W}^T \frac{\partial}{\partial p}\left(\rho c_p\right) \frac{\partial T}{\partial t}\,d\Omega + \int_{\Omega} \mathbf{W}^T \rho c_p \frac{\partial S_T}{\partial t}\,d\Omega + \int_{\Omega} \mathbf{W}^T \frac{\partial}{\partial p}\left(\rho_r c_{pr}\right)\left(\mathbf{u}\cdot\nabla T\right)\,d\Omega$$

$$+ \int_{\Omega} \mathbf{W}^T \rho_r c_{pr}\left(\frac{\partial \mathbf{u}}{\partial p}\cdot T\right)\,d\Omega + \int_{\Omega} \mathbf{W}^T \rho_r c_{pr}\left(\mathbf{u}\cdot\nabla S_T\right)\,d\Omega - \int_{\Gamma} \mathbf{W}^T \left(\frac{\partial k}{\partial p}\nabla T\cdot n\right)\,d\Gamma$$

$$+ \int_{\Omega} \nabla \mathbf{W}^T \cdot \frac{\partial k}{\partial p}\nabla T\,d\Omega - \int_{\Gamma} \nabla \mathbf{W}^T \left(k\nabla S_T\cdot n\right)\,d\Gamma + \int_{\Omega} \nabla \mathbf{W}^T \cdot k\nabla S_T\,d\Omega$$

$$- \int_{\Omega} \mathbf{W}^T \frac{\partial \Phi}{\partial p}\dot{G}\,d\Omega - \int_{\Omega} \mathbf{W}^T \Phi \frac{\partial \dot{G}}{\partial p}\,d\Omega = 0 \tag{36}$$

where ρc_p is defined in equation (2) and $\rho_r c_{pr}$ are the resin material properties. Defining that the weighting functions $\mathbf{W}$ be the SUPG weighting functions $\mathbf{N} + \lambda(\mathbf{u}\cdot\nabla\mathbf{N})$, and interpolating for T and S_T yields

$$\mathbf{W} = \mathbf{N} + \lambda(\mathbf{u}\cdot\nabla\mathbf{N})$$

$$\mathbf{T} = \sum_{i=1}^{\text{num. nodes}} W_i T_i \tag{37}$$

$$\mathbf{S_T} = \sum_{i=1}^{\text{num. nodes}} W_i S_{T_i}$$

Substituting equation (37) into equation (36), yields the semi-discretized finite element equations for the temperature CSE, given as

$$\frac{\partial \mathbf{C}}{\partial p}\dot{\mathbf{T}} + \mathbf{C}\dot{\mathbf{S}}_T + \left(\frac{\partial \mathbf{K_{ad}}}{\partial p} + \frac{\partial \mathbf{K_{cond}}}{\partial p}\right)\mathbf{T} + (\mathbf{K_{ad}} + \mathbf{K_{cond}})\mathbf{S_T} = \mathbf{S_q} + \mathbf{S_{\dot{G}}} \tag{38}$$

where each of the terms in equation (38) are defined as

$$\frac{\partial \mathbf{C}}{\partial p} = \int_{\Omega} \mathbf{W}^T \frac{\partial}{\partial p} \left(\rho c_p\right) \mathbf{N} \, d\Omega$$

$$\mathbf{C} = \int_{\Omega} \mathbf{W}^T \left(\rho c_p\right) \mathbf{N} \, d\Omega$$

$$\frac{\partial \mathbf{K_{ad}}}{\partial p} = \int_{\Omega} \mathbf{W}^T \frac{\partial}{\partial p} \left(\rho c_p\right) \left(\mathbf{u} \cdot \mathbf{B}\right) d\Omega + \int_{\Omega} \mathbf{W}^T \left(\rho_r c_{pr}\right) \left(\frac{\partial \mathbf{u}}{\partial p} \cdot \mathbf{B}\right) d\Omega$$

$$\mathbf{K_{ad}} = \int_{\Omega} \mathbf{W}^T \left(\rho_r c_{pr}\right) \left(\mathbf{u} \cdot \mathbf{B}\right) d\Omega$$

$$\frac{\partial \mathbf{K_{cond}}}{\partial p} = \int_{\Omega} \mathbf{B}_W^T \frac{\partial k_{eff}}{\partial p} \mathbf{B} \, d\Omega \tag{39}$$

$$\mathbf{K_{cond}} = \int_{\Omega} \mathbf{B}_W^T k_{eff} \mathbf{B} \, d\Omega$$

$$\mathbf{S_q} = \int_{\Gamma} \mathbf{W}^T \left(\frac{\partial k_{eff}}{\partial p} \nabla T \cdot \mathbf{n}\right) d\Gamma + \int_{\Gamma} \mathbf{W}^T \left(k \nabla S_T \cdot \mathbf{n}\right) d\Gamma$$

$$\mathbf{S_{\dot{G}\theta}} = \int_{\Omega} \mathbf{W}^T \frac{\partial \Phi}{\partial p} \dot{G} \, d\Omega + \int_{\Omega} \mathbf{W}^T \Phi \frac{\partial \dot{G}}{\partial p} \, d\Omega$$

with $\dot{G}$ defined in equation (10). The time discretization is employed as

$$\dot{\mathbf{T}}_\theta = \frac{\mathbf{T}_{n+1} - \mathbf{T}_n}{\Delta t}$$

$$\dot{\mathbf{S}}_{\mathbf{T}_\theta} = \frac{\mathbf{S}_{\mathbf{T}n+1} - \mathbf{S}_{\mathbf{T}n}}{\Delta t} \tag{40}$$

The fully discretized representations are thus given as

$$[\mathbf{C} + \theta \mathbf{K} \Delta t] \, \mathbf{S}_{\mathbf{T}_{n+1}} = - \left[\frac{\partial \mathbf{C}}{\partial p} + \theta \frac{\partial \mathbf{K}}{\partial p} \Delta t\right] \mathbf{T}_{n+1} + \left[\frac{\partial \mathbf{C}}{\partial p} - (1-\theta) \frac{\partial \mathbf{K}}{\partial p} \Delta t\right] \mathbf{T}_n$$

$$+ \left[\mathbf{C} - (1-\theta) \mathbf{K} \Delta t\right] \mathbf{S}_{\mathbf{T_n}} + \Delta t \left[(1-\theta) \frac{\partial \mathbf{F_n}}{\partial p} + \theta \frac{\partial \mathbf{F}_{n+1}}{\partial p}\right] \tag{41}$$

with temperature T and temperature sensitivity S_T approximated by

$$\mathbf{T}_\theta = (1-\theta) \mathbf{T_n} + \theta \mathbf{T_{n+1}}$$

$$\mathbf{S}_{\mathbf{T}_\theta} = (1-\theta) \mathbf{S}_{\mathbf{T_n}} + \theta \mathbf{S}_{\mathbf{T_{n+1}}} \tag{42}$$

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and **F** is defined as

$$\mathbf{F} = \mathbf{S_q} + \mathbf{S_{\dot{G}}} \tag{43}$$

Some of the terms necessary for calculating the temperature sensitivity need to be defined. The first comes from equation (3), where $\frac{\partial k_{eff}}{\partial p}$ is defined from the following equation for sensitivity parameter $p = k_r$,

$$\frac{\partial k_{eff}}{\partial p} = \frac{k_f}{k_f w_r + k_r w_f} - \frac{k_f k_r}{(k_f w_r + k_r w_f)^2} w_f \tag{44}$$

Or for $p = k_f$,

$$\frac{\partial k_{eff}}{\partial p} = \frac{k_r}{k_f w_r + k_r w_f} - \frac{k_f k_r}{(k_f w_r + k_r w_f)^2} w_r \tag{45}$$

The heat generation term, $\frac{\partial \dot{G}}{\partial p}$, is defined as

$$\frac{\partial \dot{G}}{\partial p} = H_R \frac{\partial R_\alpha}{\partial p} \tag{46}$$

where H_R is the heat of reaction per unit volume for the pure resin. The rate of reaction term, $\frac{\partial R_\alpha}{\partial p}$, is defined by

$$\begin{aligned}
\frac{\partial}{\partial p} R_\alpha = {} & \left(\frac{\partial K_1}{\partial p} + \frac{\partial K_2}{\partial p} \alpha^{n_1} + K_2 n_1 \alpha^{n_1 - 1} \frac{\partial \alpha}{\partial p} \right)(1 - \alpha)^{n_2} \\
& + (K_1 + K_2 \alpha^{n_1}) n_2 (1 - \alpha)^{(n_2 - 1)} \frac{\partial \alpha}{\partial p}
\end{aligned} \tag{47}$$

where $\frac{\partial K_1}{\partial p}$ and $\frac{\partial K_2}{\partial p}$ are found by taking the partial derivative of K_1 and K_2 in equation (12) with respect to the sensitivity parameter p, i.e.,

$$\begin{aligned}
\frac{\partial K_1}{\partial p} &= \frac{E_1 A_1}{RT^2} e^{(-\frac{E_1}{RT})} \frac{\partial T}{\partial p} \\
\frac{\partial K_2}{\partial p} &= \frac{E_2 A_2}{RT^2} e^{(-\frac{E_2}{RT})} \frac{\partial T}{\partial p}
\end{aligned} \tag{48}$$

Equation (41) is used to solve for the temperature sensitivity profile for each time step after the temperature results have been calculated.

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3.3   RTM Cure Sensitivity

In the non-isothermal RTM analysis, cure is also computed. This leads to the following evaluation of the cure sensitivity equations. The cure sensitivity equation is computed by taking the partial derivative of equation (7) with respect to the sensitivity parameter p, i.e.,

$$\frac{\partial}{\partial p}\left(\Phi\frac{\partial\alpha}{\partial t} + \mathbf{u}\cdot\nabla\alpha = \Phi R_\alpha\right) \tag{49}$$

This leads to

$$\frac{\partial\Phi}{\partial p}\frac{\partial\alpha}{\partial t} + \Phi\frac{S_\alpha}{\partial t} + \frac{\partial\mathbf{u}}{\partial p}\cdot\nabla\alpha + \mathbf{u}\cdot\nabla S_\alpha = \frac{\partial\Phi}{\partial p}R_\alpha + \Phi\frac{\partial R_\alpha}{\partial p} \tag{50}$$

where the cure sensitivity is defined as $S_\alpha \equiv \frac{\partial\alpha}{\partial p}$. Applying the method of weighted residuals, yields

$$\int_\Omega \mathbf{W}^T\left(\frac{\partial\Phi}{\partial p}\frac{\partial\alpha}{\partial t} + \Phi\frac{S_\alpha}{\partial t} + \frac{\partial\mathbf{u}}{\partial p}\cdot\nabla\alpha + \mathbf{u}\cdot\nabla S_\alpha - \frac{\partial\Phi}{\partial p}R_\alpha - \Phi\frac{\partial R_\alpha}{\partial p}\right)d\Omega = 0 \tag{51}$$

As in the temperature problem, the weighting functions $\mathbf{W}$ are defined to be the SUPG weighting functions $\mathbf{N} + \lambda(\mathbf{u}\cdot\nabla\mathbf{N})$, and interpolating for α and S_α yields

$$\mathbf{W} = \mathbf{N} + \lambda(\mathbf{u}\cdot\nabla\mathbf{N})$$

$$\boldsymbol{\alpha} = \sum_{i=1}^{\text{num. nodes}} W_i\alpha_i \tag{52}$$

$$\mathbf{S}_\alpha = \sum_{i=1}^{\text{num. nodes}} W_i S_{\alpha_i}$$

The semi-discretized cure sensitivity equation is thus given as

$$\frac{\partial\mathbf{C}}{\partial p}\dot{\boldsymbol{\alpha}} + \mathbf{C}\dot{\mathbf{S}}_\alpha + \frac{\partial\mathbf{K}}{\partial p}\boldsymbol{\alpha} + \mathbf{K}\mathbf{S}_\alpha = \frac{\partial\mathbf{Q}_{\mathbf{R}_\alpha}}{\partial p} \tag{53}$$

where the terms in equation (53) are defined as

$$\mathbf{C} = \int_\Omega \Phi \mathbf{W}^T \mathbf{N}\, d\Omega$$

$$\frac{\partial \mathbf{C}}{\partial p} = \int_\Omega \frac{\partial \Phi}{\partial p} \mathbf{W}^T \mathbf{N}\, d\Omega$$

$$\mathbf{K} = \int_\Omega \mathbf{W}^T (\mathbf{u} \cdot \mathbf{B}_N)\, d\Omega \qquad (54)$$

$$\frac{\partial \mathbf{K}}{\partial p} = \int_\Omega \mathbf{W}^T \left(\frac{\partial \mathbf{u}}{\partial p} \cdot \mathbf{B}_N \right) d\Omega$$

$$\frac{\partial \mathbf{Q_{R_\alpha}}}{\partial p} = \int_\Omega \frac{\partial \Phi}{\partial p} \mathbf{W}^T R_\alpha\, d\Omega + \int_\Omega \Phi \mathbf{W}^T \frac{\partial R_\alpha}{\partial p}\, d\Omega$$

with the time discretization employed as

$$\dot{\boldsymbol{\alpha}}_\theta = \frac{\boldsymbol{\alpha}_{n+1} - \boldsymbol{\alpha}_n}{\Delta t}$$

$$\dot{\mathbf{S}}_{\alpha_\theta} = \frac{\mathbf{S}_{\alpha_{n+1}} - \mathbf{S}_{\alpha_n}}{\Delta t} \qquad (55)$$

The cure sensitivity is solved numerically employing

$$[\mathbf{C} + \theta \mathbf{K} \Delta t]\, \mathbf{S}_{\alpha_{n+1}} = - \left[\frac{\partial \mathbf{C}}{\partial p} + \theta \frac{\partial \mathbf{K}}{\partial p} \Delta t \right] \boldsymbol{\alpha}_{n+1} + \left[\frac{\partial \mathbf{C}}{\partial p} - (1 - \theta) \frac{\partial \mathbf{K}}{\partial p} \Delta t \right] \boldsymbol{\alpha}_n$$
$$+ \left[\mathbf{C} - (1 - \theta)\mathbf{K} \Delta t \right] \mathbf{S}_{\alpha_n} + \Delta t \left[(1 - \theta) \frac{\partial \mathbf{F_n}}{\partial p} + \theta \frac{\partial \mathbf{F}_{n+1}}{\partial p} \right] \qquad (56)$$

with cure α and cure sensitivity S_α approximated by

$$\boldsymbol{\alpha}_\theta = (1 - \theta)\boldsymbol{\alpha}_n + \theta \boldsymbol{\alpha}_{n+1}$$

$$\mathbf{S}_{\alpha_\theta} = (1 - \theta)\mathbf{S}_{\alpha_n} + \theta \mathbf{S}_{\alpha_{n+1}} \qquad (57)$$

All of the terms in equation (56) are defined in equations (26) and (54).

3.4 Computational Procedure

The 14 steps required to perform the sensitivity analysis for non-isothermal RTM process modeling are outlined next.

1. The filling analysis is described by the following semi-discretized equation:

$$\mathbf{KP} = \mathbf{q} \tag{58}$$

2. For non-isothermal filling analysis include the necessary temperature, equation (19), and the cure equation, equation (25).

3. The CSE for the RTM filling simulation is given in semi-discretized form in equation (28).

4. For the non-isothermal sensitivity analysis, it is also necessary to take the partial derivative of the temperature and cure equations with respect to the sensitivity parameter p, equations (33) and (49). This results in the semi-discretized equations for temperature and cure, equations (38) and (53), respectively.

5. To solve the filling equation, the boundary conditions are defined as

$$\frac{\partial P}{\partial \mathbf{n}} = 0 \text{ on mold walls}$$

$$P = 0 \text{ at flow front}$$

$$P = P_0 \text{ prescribed pressure at inlet} \tag{59}$$

$$\text{or}$$

$$q = q_0 \text{ prescribed flow rate at inlet}$$

6. To solve the filling sensitivity equations, the boundary conditions need to be computed

by taking the partial derivatives of all filling boundary conditions given as

$$\frac{\partial}{\partial p}\left(\frac{\partial P}{\partial \mathbf{n}}\right) = 0 \text{ on Mold Walls}$$

$$\frac{\partial P}{\partial p} = 0 \text{ at flow front}$$

$$\frac{\partial P}{\partial p} = \frac{\partial P_0}{\partial p} \text{ for constant pressure at inlet} \tag{60}$$

or for constant flow at the inlet

$$\frac{\partial q}{\partial p} = \frac{\partial q_0}{\partial p} \text{ for constant flow rate at inlet}$$

7. For the non-isothermal analysis, the temperature and cure boundary conditions are required and are defined in equations (5) and (8), respectively.

8. For temperature and cure sensitivities, the thermal boundary conditions need to be computed. The temperature sensitivity boundary conditions can be found in equation (35), with the cure sensitivity boundary conditions defined at the inlet as $S_\alpha = 0$.

9. For the non-isothermal RTM sensitivity analysis, $\frac{\partial \mathbf{K}}{\partial p}$ and $\mathbf{S}_q$ must be computed and boundary conditions applied. The matrix $\frac{\partial \mathbf{K}}{\partial p}$ requires $\frac{\partial \mathbf{K}}{\partial p}$ and $\frac{\partial \mu(T,\alpha)}{\partial p}$ as defined in equation (31). The values in vector $\mathbf{S}_q$ are set to zero, except where the inlet flow rate has been defined.

10. The temperature sensitivity analysis requires computation of five matrices and vectors including, $\frac{\partial \mathbf{C}}{\partial p}$, $\frac{\partial \mathbf{K}_{\mathbf{ad}}}{\partial p}$, $\frac{\partial \mathbf{K}_{\mathbf{cond}}}{\partial p}$, $\mathbf{S}_{\mathbf{q}}$, and $\mathbf{S}_{\dot{\mathbf{G}}}$. The values required for all of these terms can be found in equation (39).

11. Similarly, for the cure sensitivity, $\frac{\partial \mathbf{C}}{\partial p}$, $\frac{\partial \mathbf{K}}{\partial p}$, and $\frac{\partial \mathbf{Q}_{\mathbf{R}\alpha}}{\partial p}$ are required and are defined in equation (54).

12. Once all of these equations are defined and the boundary conditions applied, the results must be obtained. First the pressure results are computed, followed by the pressure sensitivity results. After the filling is completed for the current time step, the thermal computations are performed. The temperature and cure considerations are obtained

first, followed by the temperature and cure sensitivities. Note that the temperature and cure time step is normally less than the filling time step (see Ngo et al. [9]).

13. Before continuing on to the next filling step, compute the new viscosity and viscosity sensitivity values from the thermal results and reform $\mathbf{K}$ and $\frac{\partial \mathbf{K}}{\partial p}$.

14. Proceed to the next filling time step until the mold is completely filled.

3.5 Example Geometry With Numerical Results

An axi-symmetric example geometry is shown in Figure 1. The disk is filled with inlets placed along the inside radius of the disk. By varying the inlet boundary conditions and the material properties, it is possible to show how these variables affect the fill time or inlet pressure of the model. Observation of the results of the sensitivity values for these variables are used to indicate the qualitative and quantitative changes these variables produce. The results presented in Figures 2–5 are obtained with the geometry and mesh shown in Figure 1.
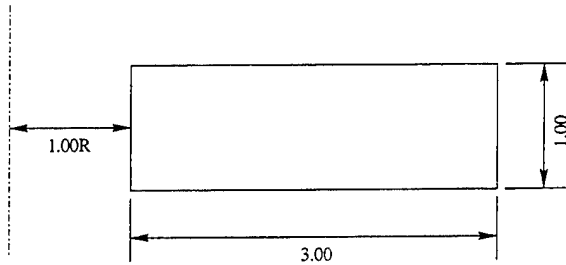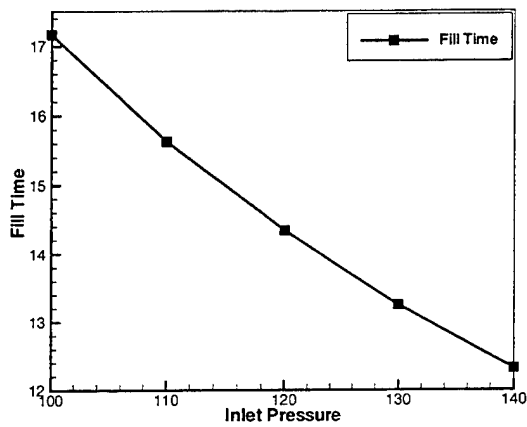
(a) 4.00-in. R disk with 1.00-in. R hole for non-isothermal RTM study
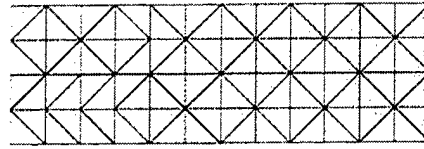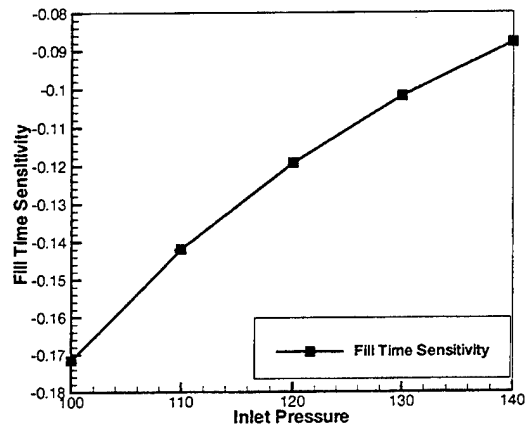
(b) Mesh of 4.00-in. R disk with 1.00-in. R hole

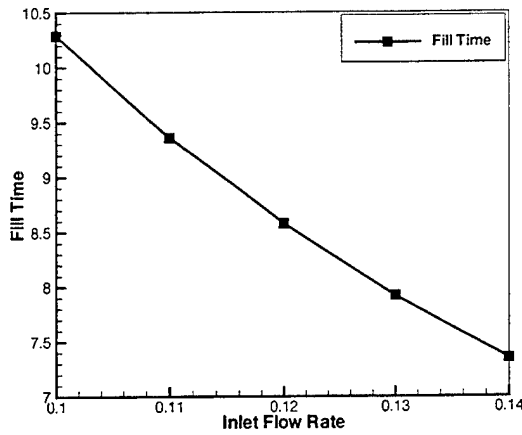Figure 1: Example geometry and finite element mesh.
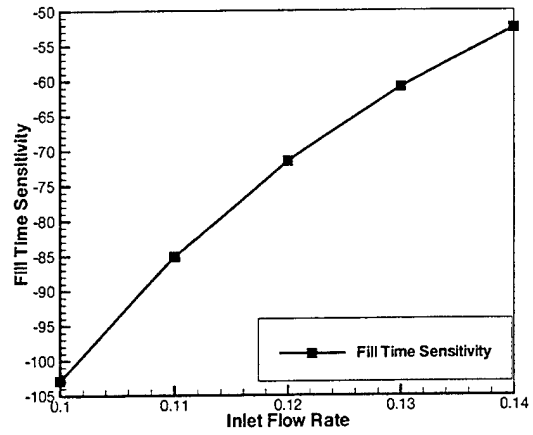

(a) Non-isothermal fill time vs. inlet pressure

(b) Non-isothermal fill time sensitivity vs. inlet pressure

Figure 2: Non-isothermal fill time and fill time sensitivity vs. inlet pressure plots for the 4.00-in. R disk model.
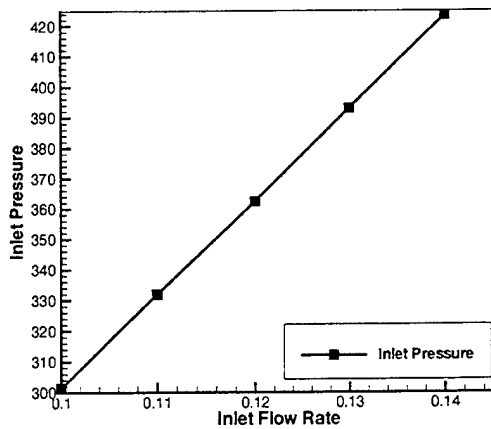
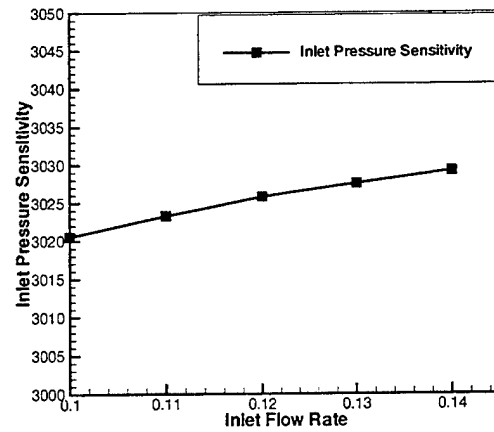(a) Non-isothermal fill time vs. inlet flow rate

(b) Non-isothermal fill time sensitivity vs. inlet flow rate

Figure 3: Non-isothermal fill time and fill time sensitivity vs. inlet flow rate plots for the 4.00-in. R disk model.
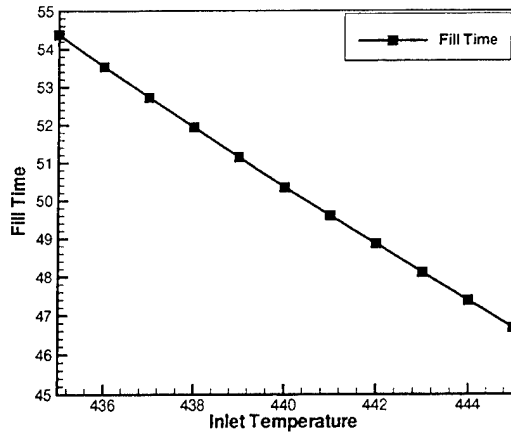

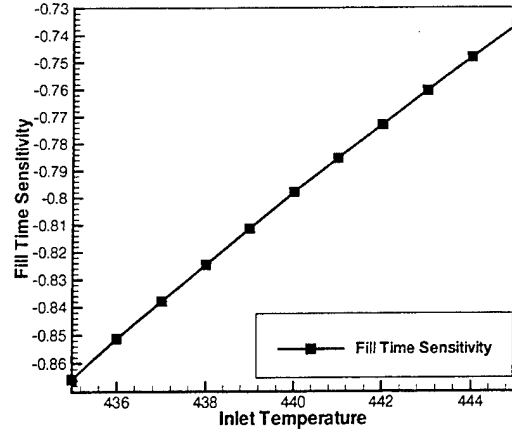(a) Non-isothermal inlet pressure vs. inlet flow rate

(b) Non-isothermal inlet pressure sensitivity vs. inlet flow rate

Figure 4: Non-isothermal inlet pressure and inlet pressure sensitivity vs. inlet flow rate plots for the 4.00-in. R disk model.

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(a) Non-isothermal fill time vs. inlet temperature

(b) Non-isothermal fill time sensitivity vs. inlet temperature

Figure 5: Non-isothermal fill time and fill time sensitivity vs. inlet temperature plots for the 4.00-in. R disk model.

Figure 2 shows plots of the fill time and the fill time sensitivity versus inlet pressure. These results demonstrate that the fill time decreases with increasing inlet pressure, which follows the trend observed in the analytical solution for isothermal considerations as given by

$$t = \frac{\mu}{k}\frac{\Phi}{P_0}\left[\frac{R^2}{2}ln\left(\frac{R}{R_0}\right) - \frac{R^2}{4} + \frac{R_0{}^2}{4}\right] \tag{61}$$

where

$$\mu = \text{viscosity}$$

$$\Phi = \text{porosity}$$

$$k = \text{permeability}$$

$$P_0 = \text{Inlet Pressure}$$

$$R_0 = \text{Inner Radius}$$

$$R = \text{Outer Radius}$$

$$t = \text{Time to fill from } R_0 \text{ to } R$$

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Figure 3 shows the fill time and the fill time sensitivity versus inlet flow rate. The results are as expected since the volume of the mold remains constant; and, the fill time decreases as inlet flow rate increases. Figure 4 is a plot of pressure at the mold inlet with respect to the inlet flow rate; it shows that inlet pressure is approximately a linear function of the inlet flow rate for the given range of values. Figure 5 shows results unattainable from isothermal analysis. From the numerical results it is possible to plot the fill time and the fill time sensitivity versus inlet temperature. As expected, the fill time decreases as the inlet temperature increases because viscosity is a function of temperature, and the viscosity decreases with increasing temperature. Hence, from the isothermal analytical solutions, one observes that as the viscosity decreases for a constant inlet pressure, so does the mold fill time. All of these results follow what is expected from experience and from representative isothermal analytical solutions. The sensitivity results also follow the expected trends for the specified boundary conditions.

3.6 Verification of Non-Isothermal RTM Sensitivity Equations

Since there does not exist an available analytical solution for the non-isothermal filling process, the following definition of the derivative is employed:

$$\lim_{\Delta p \to 0} \frac{t_{fill}(p + \Delta p) - t_{fill}(p)}{\Delta p} = \frac{\partial t_{fill}}{\partial p} = S_{t_{fill}} \tag{62}$$

The associated error calculation is taken as

$$\text{Error} = \frac{\Delta p \cdot S_{t_{fill}}}{t_{fill}(p + \Delta p) - t_{fill}(p)} - 1.0 \tag{63}$$

where p and Δp are the value of the sensitivity parameter and the change in the sensitivity parameter, respectively (e.g., T_{inlet}). For verification purposes, the error, as defined in equation (63), should monotonically approach zero as Δp decreases. Also, the results obtained

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from a Taylor series expansion, equation (64), should closely follow the numerical results for small changes in the sensitivity parameter, or graphically these results should be tangent to the solution of the numerical analysis obtained by employing repeated numerical simulations.

The first order Taylor series expansion is given as

$$w(p) = w(p_0) + \frac{\partial w}{\partial p}|_{p_0}(p - p_0) + \cdots \tag{64}$$

where $w(p)$ is the numerical result and p is the sensitivity parameter. Note that the non-isothermal model verification in this section refers to the axi-symmetric model shown in Figure 6(a), with the following parameters:

$$T_{mold} = 450.00°F$$

$$\Delta t = 0.01s$$

$$k = 5.300 \cdot 10^{-6} in^2$$

$$P_0 = 300.00psi$$

Since the focus of this work is non-isothermal RTM process modeling sensitivity, the verification is only performed here for the thermal sensitivity parameter of inlet temperature. For the verification of the inlet temperature sensitivity parameter, the Taylor series is used to compare the sensitivity results to the derivative of the fill time with respect to the inlet temperature. The original Taylor series assumed for estimating the fill time results is shown here as

$$t_{fill_1} = t_{fill_0} + \frac{\partial t_{fill}}{\partial T_{inlet}} \cdot \Delta T_{inlet} \tag{65}$$

In the first-order Taylor series estimation from equation (65), the resin viscosity is not explicitly included. The viscosity term is instead encapsulated inside the fill time sensitivity term, $\frac{\partial t_{fill}}{\partial T_{inlet}}$, in equation (65). Viscosity is a function of the temperature profile inside of the part, which in turn is a function of the inlet temperature. This dependence of the
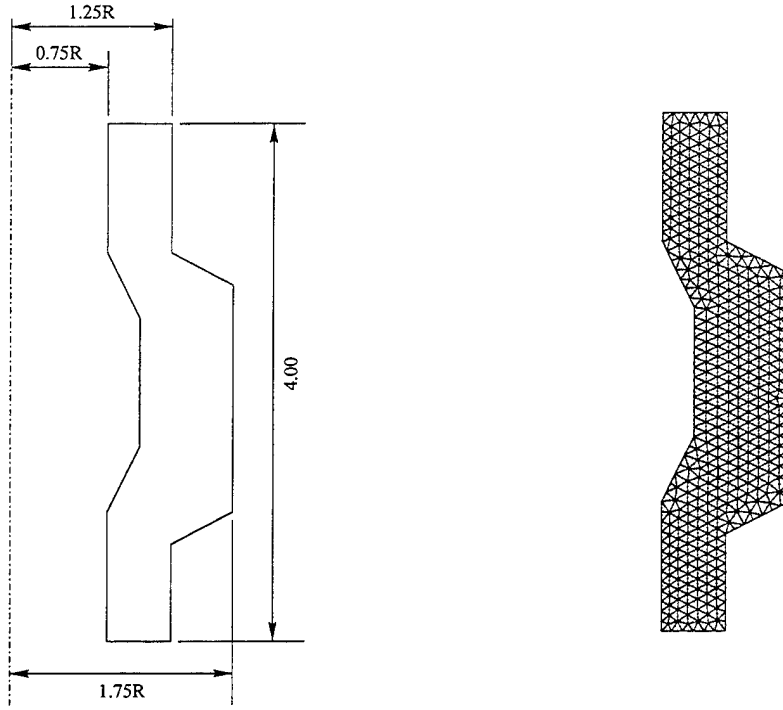
(a) Axi-symmetric part for verification study of non-isothermal RTM

(b) Axi-symmetric part mesh for verification study of non-isothermal RTM

Figure 6: Geometry and finite element mesh used for analytical/numerical comparison.

temperature profile on the inlet temperature gives the viscosity term a reliance on inlet temperature which is used to define a new Taylor series dependent on viscosity. In order to explicitly list the viscosity in the Taylor series expansion, the following modified Taylor series is used, which is based on the viscosity sensitivity.

$$t_{fill_1} = t_{fill_0} + \frac{\partial t_{fill}}{\partial \mu} \cdot \Delta \mu \tag{66}$$

The $\Delta \mu$ term is computed for every filled node in the numerical model at each filling time step. The final $\Delta \mu$ used in the Taylor series is a weighted average of each time step, weighted by the volume filled at the respective time step. The reason for using the fill time sensitivity with respect to viscosity is that the fill time is a direct function of viscosity rather than

inlet temperature. This fact is reflected in the calculations performed, where viscosity is the only filling parameter calculated with the results from the thermal analysis. The new method described by equation (66) for estimating the fill times shows reduced error with the modification presented when compared to the method from equation (65), for multiple temperature ranges. The results using equation (65) and equation (66) are shown graphically in Figures 7, 8, and 9 for inlet temperatures of 300°, 350°, and 420°, respectively. In the legends, T_{inlet} refers to the Taylor series initially used for the error estimation, and Visco. and T_{inlet} refers to the modified Taylor series estimation. The lines representing the viscosity based estimations more closely follows the finite element results than the lines representing the Taylor series estimation with inlet temperature only. It is observed that the viscosity and inlet temperature line does not always fall below the finite element results, i.e., tangent to the results curve. This error is explained by the fact that the filling calculation is dependent on the resin viscosity, which is in turn dependent on the calculated temperature profile.
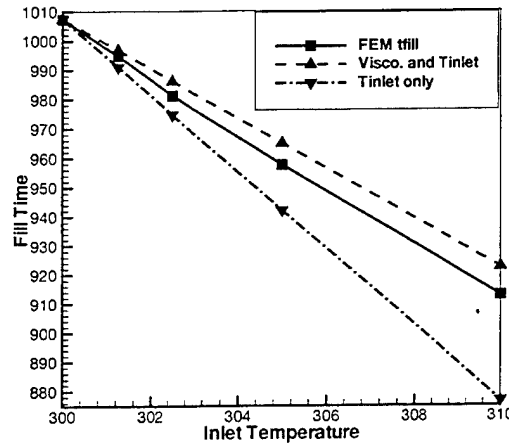

Figure 7: Comparison of the two methods for estimating fill time for $T_{inlet} = 300.0°F$, for the axi-symmetric verification model.
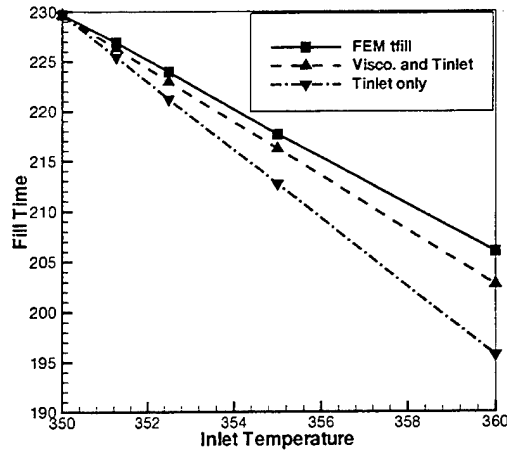
Figure 8: Comparison of the two methods for estimating fill time for $T_{inlet} = 350.0°F$, for the axi-symmetric verification model.
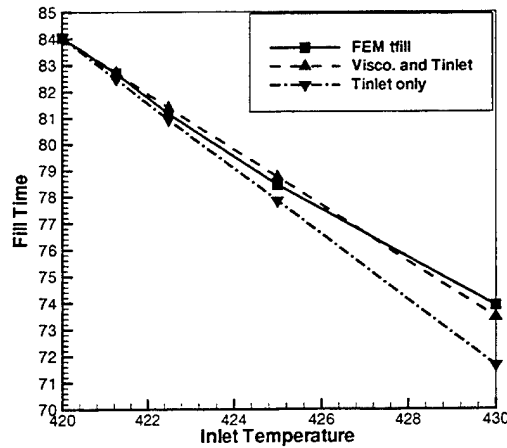

Figure 9: Comparison of the two methods for estimating fill time for $T_{inlet} = 420.0°F$, for the axi-symmetric verification model.

4. Concluding Remarks

In this report, the continuous sensitivity equation has been developed for non-isothermal considerations in RTM process modeling. This includes the non-isothermal RTM filling CSE,

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the temperature CSE, and the cure CSE. Sensitivity parameters have been examined for the cases of material properties, boundary conditions, and geometric parameters. Numerical results were presented for an example axi-symmetric model and discussed. Finally, the fill time sensitivity results for the non-isothermal resin transfer molding numerical model were verified. This was accomplished by modifying the Taylor series initially used to estimate the fill time for small changes in inlet temperature as given in equation (65), with the modified Taylor series given in equation (66). The results using the modified Taylor series indicate that the dependence of fill time on inlet temperature is not direct but rather is a side effect of changes in viscosity.

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13. ABSTRACT *(Maximum 200 words)*

The resin transfer molding (RTM) manufacturing process consists of either of two considerations. The first is the fluid flow analysis where tracking of the flow fronts are of primary importance, and the second is the combined multi-disciplinary flow/thermal analysis, where kinetics and cure need to be accounted for in the process modeling stages. In the combined multi-disciplinary flow/thermal analysis, viscosity is a function of temperature. The so-called continuous sensitivity formulations are developed for the latter case of non-isothermal process modeling of composites manufactured by RTM to predict, analyze, and optimize the manufacturing process. Attention is focused on developments for non-isothermal process modeling simulations, and numerical illustrative examples are presented for the sensitivity analysis of structural composites manufactured by RTM.

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